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13. ABSTRACT (Maximum 200 words)

This workshop is co-sponsored by the National Science Foundation, the Army Research Office, the US Association for Computational Mechanics, the Oak Ridge National Laboratory – Fusion Materials Program. It provides a forum to assess the status of computational nanomechanics research and education, and serves to educate junior researchers (primarily junior faculty members) in this emerging field. In addition to the education provided, the workshop has also resulted in several recommendations of future research directions. The recommended focuses of future research are: (1) integration of nanostructure elements and the accompanying nanomechanics; (2) the issue of multiple time scales in nanomechanics; (3) nanomechanics of the interface between soft biological systems and harder solid structures at the nanoscale, and (4) cross fertilization of physics, chemistry, materials science, continuum mechanics, and computation.

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Computational Nanomechanics of Materials

Cross Fertilization of Physics, Chemistry, Materials Science, Mechanics, and Computation

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I wish to thank my co-organizers (KJ Cho, Jacob Fish, and Wing Kam Liu) and all the participants for their contribution. In particular, I thank Ken Chong and Wing Kam Liu for their guidance and help in coordinating with the NSF Summer Institute on Nano Mechanics and Materials.

The views, opinions, and/or findings contained in this report are those of the authors/participants and should not be construed as an official National Science Foundation or Department of the Army position, policy, or decision, unless so designed by other documentation.

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Executive Summary

Computational nanomechanics is an emerging field that exists at the union of traditionally independent research areas, spanning not only computation and mechanics, but also physics, chemistry, and materials science. This interdisciplinary nature calls for cross fertilization between these many research areas. As a vital element of nanotechnology, computational nanomechanics must become a core feature of future curricula of engineering schools.

The USACM workshop on computational nanomechanics (sponsored by NSF, ARO, USACM, and ORNL-FMP) took place in Chicago on April 26 and 27, 2004. The workshop consisted of a tutorial session of six lectures, one panel session on nanomechanics research, one panel session on nanomechanics education, and one poster session. The two main topics of this workshop were education and research in nanomechanics. Reflecting the education facet were the lectures for junior scientists and the panel discussion on curriculum development. The research facet, as reflected through both lecture and panel discussion formats, emphasized complementing coverage of various length and time scales involved in nanomechanics.

In addition to providing a platform for scientific exchanges, this workshop also focused on the assessment of computational nanomechanics on education and research, and made recommendations to government agencies and the community at large. The following are recommendations from the group of workshop participants:

- Education in nanomechanics should be incorporated into existing engineering curricula instead of standing alone in new and separate elective courses.
- Integration of nanostructure elements and the accompanying nanomechanics are important to emerging nanotechnology, and its research and development deserves a concerted effort within the academic community and beyond.
- The issue of multiple time scales in nanomechanics has not received as much attention as that of multiple length scales, and should be a focus of future studies.
- Nanomechanics of the interface between soft biological systems and harder solid structures at the nanoscale is important scientifically, and its study may also lead to solutions to pressing energy issues.
- Nanomechanics research is most fruitful through sincere *cross fertilization of physics, chemistry, materials science, continuum mechanics, and computation*.

1. Background of the Workshop

The workshop on Computational Nanomechanics of Materials took place to address the need of cross fertilization among researchers in computation, physics, chemistry, materials, and mechanics, as well as the importance of incorporating nanomechanics in engineering curricula. In comparison to other mechanics workshops/symposia (Ghoniem, Busso, and Huang 2003; Campbell et al 1998), this workshop focuses on cross fertilization in both research and education.

Cross fertilization has always been a goal in science, and it is an absolute necessity in computational nanomechanics. Historically, cross fertilization emerged in the field of nanoscale mechanics, which emphasizes dislocations, earlier than in mechanics of nanostructures. Along each of the two branches – nanoscale mechanics and mechanics of nanostructures, research has progressed in an interdisciplinary manner at various levels. The following paragraphs offer a glimpse of the interdisciplinary nature in terms of computation and mechanics, and their interface with materials and physics and chemistry.

Scale bridging methods in computational mechanics go back more than 30 years (see Mote 1971). For review article on various efforts in mid and late 70s see Noor (1988) and Dong (1983). In 80s and 90s various Local Enrichment Methods (LEM) where the fine scale function were used to embed discontinuities (Belytschko 1988; Fish and Belytschko 1988; Belytschko and Fish 1989; Armero and Garikipati 1996; Simo et al 1993) became very popular. Variational Multiscale Method (VMS) (Hughes 1995) and Mathematical Homogenization (Babuska 1975; Benssousan et al 1978; Guedes and Kikuchi 1990) fall into this category of methods. An attractive feature of these methods is that fine-scale features can be eliminated either on the coarse scale element level or at the coarse scale material point resulting in embedded fine-scale physics at the coarse scale without significantly increasing the cost of coarse scale computations. In LEM fine scale features are only approximated, and their gross response is injected into the coarse scale. The need to control fine scale approximations without compromising the sparsity of discrete approximations produced several enrichment schemes including the s-version of the finite element method (Fish 1992; Fish and Markolefas 1993; Fish et al 1994; Park et

al 2003), various multigrid-like scale bridging methods (Fish and Belsky 1995a and 1995b; Fish et al 1997), the Extended Finite Element Method (XFEM) (Belytschko and Black 1999; Moës et al 1999; Belytschko et al 2001), and the Generalized Finite Element Method (GFEM) (Strouboulis et al 2000 and 2001) both based on the Partition of Unity (PU) framework (Babuska et al 1994; Babuska and Melenk 1996) and the Discontinuous Galerkin (DG) (Oden et al 1998; Fish and Chen 2004) method. The multiscale methods based on the concurrent resolution of multiple scales are often called as embedded or concurrent.

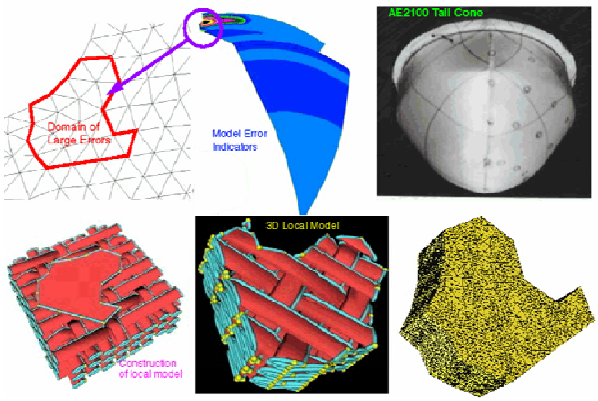

Figure 1: Application of multigrid-like method in design (Courtesy of Jacob Fish).

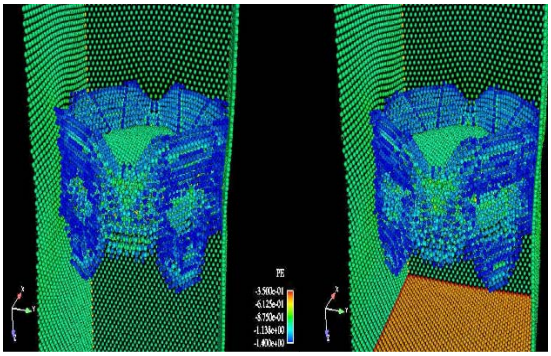

Figure 2. Crack branching MD (left) and MD/FEM bridging scale (right) simulation; Courtesy of Wing Kam Liu.

Many of the multiscale technologies developed for bridging continuum scales can be applied to bridging discrete and continuum scales often needed in nanotechnology applications. Notable examples are some multigrid-like procedures (Fish and Chen 2004; Wagner and Liu 2003; Datta et al 2004) (see Figure 1), generalized mathematical homogenization theory (Fish and Schwob 2003), overlapping domain decomposition (Belytschko and Xiao 2003), bridging scale (McVeigh and Liu 2004; Karpov et al. 2004 – see Figure 2) and multiscale enrichment based on partition of unity method (Fish and Yuan 2004).

In parallel to the advancement of computational methods, physical principles of nanomechanics have been sought after continuously through the years. Defects such as

dislocations may be accounted for through gradients of strains (Fleck and Hutchinson 1993), or directly through the dislocation elastic fields (Canova et al 1992; 1993; Huang and Ghoniem 2003; Zbib et al 1996; Rhee et al 1998). Away from the cores of dislocations, linear elasticity works fine and the continuum models usually suffice. Near the cores, nonlinear and non-plastic fields require atomistic descriptions. Driven by this duality of dislocation fields, several approaches toward modeling the mechanics of materials have been developed around embedding atomistic regions into a continuum (Shenoy et al 1999; Abraham et al 1998). As shown in Figure 3, a crack, whose propagation usually accompanies dislocation emissions, is represented by a pileup of point-like atoms. At the crack front, the atoms are composed of nuclei and electrons, the latter being treated using methods derived from quantum mechanics. Directly embedding atomic (and electronic) regions in a continuum is attractive when few dislocations are involved and when long-range strain fields are important. In parallel, large scale atomistic simulations (Figure 4) are advantageous in studying interactions of many dislocations.

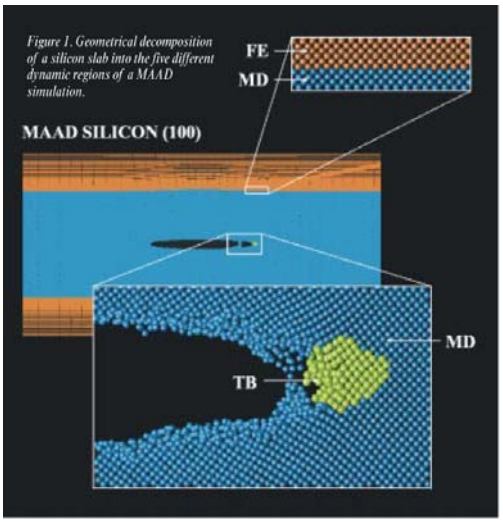

Figure 3: Quantum mechanical, atomistic, and continuum descriptions of a propagating crack; Source: Abraham et al 1998.

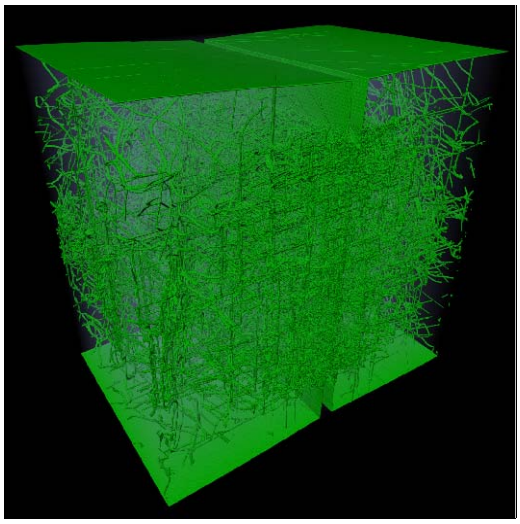

Figure 4: Dislocations around cracks – billion atoms simulation; Source: Abraham, Duchaineau, and Diaz De La Rubia, www.llnl.gov/largevis/atoms/ductile-failure.

The long-range strain fields of multiple dislocations are partially shielded by each other and simple boundary conditions usually would suffice for mechanistic investigations. In more rigorous atomistic simulations, the long-range effects are treated through the application of the Green's function method (Golubov et al 2001). Similar simulations are also applicable to point defects, interfaces, twinning, and crystal phase transformations (Yip et al 2001). The advancement in modeling nanoscale mechanics (or dislocation mechanics) relies on interactions across the disciplines of continuum mechanics, physics of atoms and electrons, and computation in a parallel computing environment.

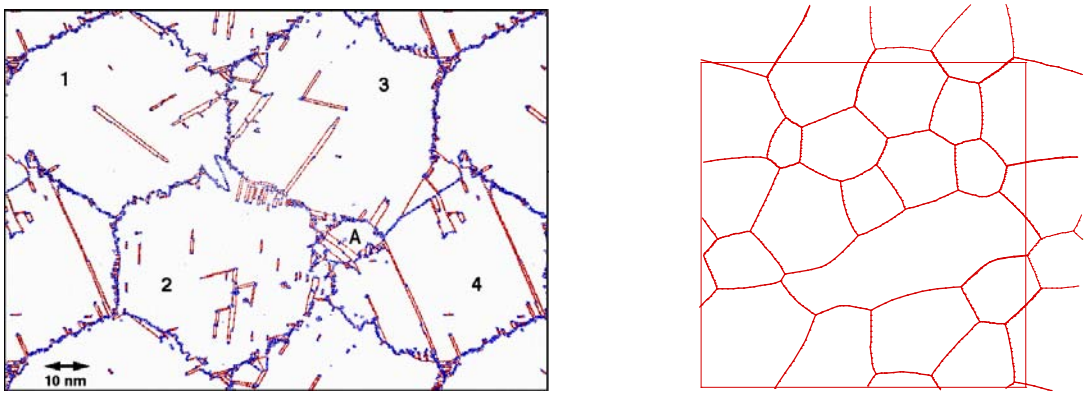

Figure 5: Nanograin simulations at the atomic (left) and mesoscopic (right) levels; Source: Dieter Wolf's presentation in this workshop.

From nanoscale mechanics to mechanics of nanostructures, the focus shifts from dislocations to nanoscale structures. The first example is the transition from microscale polycrystals to nanograins. At the microscale, each grain in a polycrystal deforms through primarily dislocation activities. Through dislocation mechanics, strain gradient plasticity, and homogenization, the deformation can be modeled accurately. However, at the nanoscale (<100 nm), the deformation mechanisms change and grain boundary activities contribute substantially to the plastic deformation. As a result, the Hall-Petch relationship that governs the dislocation hardening in microscale polycrystals is inverted (Nieh et al 1997). More interestingly, the seemingly unlikely deformation mechanism – twinning in face-centered-cubic metals (Figure 5 left) – becomes active in nanograins (Yamakov et al

2002; 2003). The new deformation mechanisms are identifiable through atomistic simulations. However, their impacts on materials at technologically relevant dimensions cannot be predicted by the atomistic simulations alone. Continuum models (Figure 5 right) that take into account of the new mechanisms are needed and are being developed (Moldovan, Wolf and Phillpot, 2003). As a result of this interdependence, the computational mechanics of nanograins links the physics of atoms and the mechanics of large scale continuum.

Next to nanograins, nanotubes form an entirely different group of nanostructures. And their mechanics has been modeled at quantum mechanical, atomistic, and continuum levels. Based on quantum mechanics simulations, mechanical deformation changes the electronic structure of a nanotube and converts a semi-conducting nanotube to a conducting one (Peng and Cho 2002). Further increase of the mechanical deformation, as revealed by atomistic simulations, leads to propagation of Stone-Wales defects resembling the dislocation glide in crystals and to buckling of macroscopic shells (Figure 6 left). This behavior is affected by the addition of chemical molecules (Figure 6 right), demonstrating the coupling of chemistry and mechanics. Adding cages like C_{60} molecules in a large nanotube may produce nanoscale pistons, and adding smaller nanotubes may result in wearless nanoscale bearings (Qian et al. 2001).

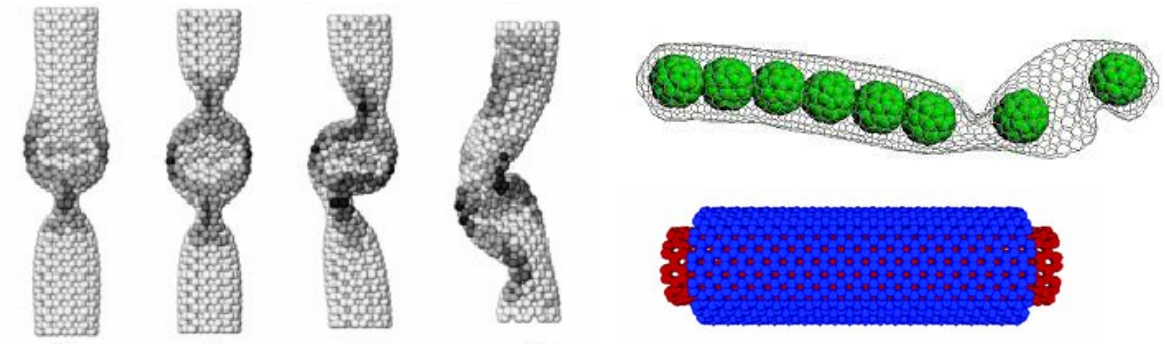

Figure 6: Deformation of nanotubes without (left) and with molecules (upper right) or another tube (lower right); Source: Yakobson et al 1996 (left) and Ni et al 2002 (upper right), and Wing Kam Liu (lower right).

Efforts have been made to incorporate the atomic level deformation mechanism with continuum models (Arroyo and Belytschko 2002; 2003). However, it is not always so clear how to link atomic and continuum quantities. For example, the thickness of a nanotube wall is only one atomic layer, and its thickness is by no means unambiguously defined. The modeling of deformation mechanisms of nanotubes and their chemical interactions with molecules requires a combination of chemistry and physics. Extending the models to large stack of nanotubes requires additional branches of study: computation and mechanics.

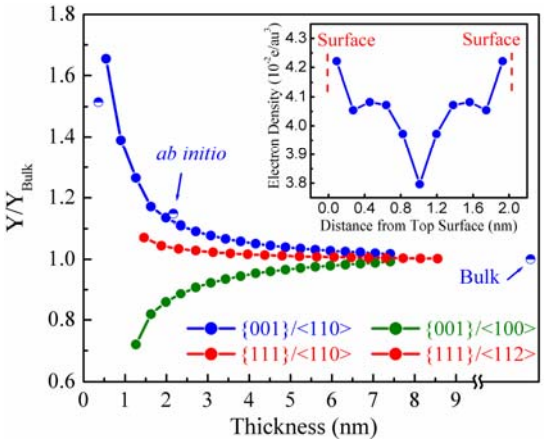

Figure 7a: Normalized Young's moduli vs thickness of Cu nanoplates; Source: Zhou and Huang 2003.

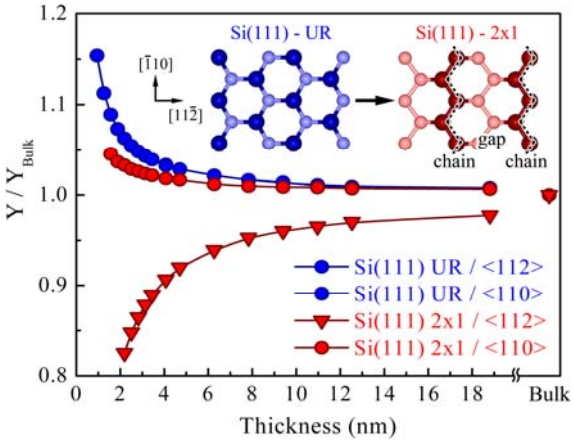

Figure 7b: Normalized Young's moduli vs thickness of Si nanoplates; Source: Shim, Zhou, Huang, and Cale 2004.

In between nanotubes and nanograins are nanoplates, and their one-dimensional equivalent, nanobeams. A nanoplate (nanobeam) is a crystal that is small in one (two) direction. Because of the small dimension, both elastic and plastic deformations are unique in comparison to their counterparts of large single crystals. It is easy to conceive that the elastic constant of a nanoplate is smaller than its bulk value. However, it may be counterintuitive to imagine the opposite. A combination of quantum mechanical and atomistic simulations show that the elastic constant of a nanoplate can be larger or smaller than the corresponding bulk value; Figure 7a. For covalent nanoplates, surface

reconstruction may reverse the stiffening behavior' Figure 7b. The variation is the result of competition among bond loss, bond saturation, and reconstruction on solid surfaces (Zhou and Huang 2003; Shim et al 2004). As the mechanical load increases beyond the elastic domain, phase transformation takes place before dislocations glide as in bulk crystals (Diao et al 2003). The quantum mechanical and atomistic models suffice in most single elements of nanobeams or nanoplates. On the other hand, technologically relevant structures involve more than a single element. The modeling of a large number of nanoplates and nanobeams (possibly together with nanotubes and other structures) is beyond the capacity of the rigorous quantum mechanical and atomistic models. Continuum mechanics models that take into account of the atomic and electronic mechanisms – such as bond saturation and phase transformation at surfaces – are necessary, and they are in general unavailable, although efforts are underway.

The aforementioned multiscale modeling of nanomechanics focuses primarily on the length scale. During materials fabrication, the time scale becomes extremely important. For example, strain of magnitude 0.7% may develop during thin film deposition (Huang et al 2003). The strain evolution depends on many fast processes, such as dislocation nucleation from surfaces (Liu et al 2002), which take place over pico-seconds. On the other hand, a materials fabrication process takes much longer. A typical thin film deposition process would take minutes. The details of atomic processes – atomic vibration, diffusion, and displacement associated with dislocation activities – must be incorporated in modeling the materials fabrication (Huang 2004; Huang, Gilmer, and Diaz de la Rubia 1998). Some of the approaches have been described in the Handbook of Multiscale Materials Modeling (Yip 2004).

In contrast to the rich development in computational nanomechanics research, the progress of computational nanomechanics education has been limited. Several universities have introduced graduate-level courses carrying the word "nanomechanics" in the title. However, it has not been demonstrated clearly how computational nanomechanics of materials, or more broadly, nanomechanics, will be incorporated into undergraduate curricula. Traditionally, mechanics is an element of mechanical and civil engineering departments. Taking a nanomechanics course, a student must have a

combined background of traditional continuum mechanics, materials science, physics, and chemistry. Because of this interdisciplinary nature, it is a challenge to fit a nanomechanics course into a particular engineering program.

The glimpse of the past developments reveals the necessity of addressing the interdisciplinary research and education of computational nanomechanics. Such effort will benefit not only scientific advancement (presentation of Ken Chong in this workshop), but also national defense (presentation of Bruce LaMattina in this workshop), homeland security (presentation of Tomas Diaz de la Rubia in this workshop), energy development (presentation of Stephen Zinkle, in this workshop), and emerging nanotechnology (presentation of Max Lagally in this workshop).

2. Description of the Workshop

This workshop has three elements: a lecture session, two panel discussion sessions, and a poster session. The lectures cover the topic of computational nanomechanics from combined perspectives of physics, chemistry, materials, and computational mechanics. They serve the purpose of (1) providing an overview of computational nanomechanics from various perspectives, and (2) providing background education to junior researchers (primarily junior faculty members) on this interdisciplinary subject. Five lectures are offered. The lecture of Jacob Fish focuses on the state-of-the-art computational methods with a look forward look toward excitements and difficulties. The lecture of Sidney Yip illustrates the use of quantum mechanics and classical molecular dynamics in nanomechanics of crystals, such as phase transition under stress and dislocation activities. Turning to nanostructures, the lecture of Donald Brenner covers the atomic level researches on mechanics of nanotubes, including single nanotubes and those surrounded by chemical and biological molecules. Continuing the topic of nanostructures, Dieter Wolf presents an atomic level understanding of nanograins mechanics, and the current status of incorporating atomic mechanisms in continuum models. Following the three lectures on individual nanomechanics topics, Wing Kam Liu presents the current multiscale modeling approaches in linking the

physics/chemistry/materials understanding with continuum models. The final lecture, by Max Lagally, demonstrates the driving force of computational nanomechanics – the emerging nanotechnology.

The lectures are followed by two panel discussions, which focus on where the computational nanomechanics should go in the future. The first panel – led by George Dvorak, Zdenek Bazant, and Ted Belytschko (secretary: Lucy Zhang) – focuses on the scientific aspect of the computational mechanics. In particular, the panel identifies outstanding issues and recommends mechanisms to tackle them. The second panel – led by Tomas Diaz de la Rubia, Bruce LaMattina, Steve Zinkle, and KJ Cho (secretary: Catalin Picu) – focuses on the broader impacts of computational nanomechanics. In particular, the panel discusses and identifies the need for computational nanomechanics in national defense, homeland security, energy production, and education of students. Small group discussions that follow the panel discussions further elaborate the pressing issues of research (led by Sidney Yip) and education (led by Suvranu De and Wilkins Aquino).

The poster session provides a platform for junior researchers to showcase their recent developments on the subject of computational nanomechanics. The posters cover a broad range of topics, from nanoplates to nanotubes and to nanoscale mechanics.

A list of workshop participants is available at the end of this report. And the CD also contains a complete set of lecture notes and panel discussion slides.

3. Outcome of the Workshop

This workshop provides an interdisciplinary environment for researchers to interact and to learn. The first result is the education of junior researchers (primarily junior faculty members). The lectures and discussions serve to prepare the junior researchers for their research, and for their roles in educating the nation's students in computational nanomechanics. The second result is the cross-fertilization of researchers in physics, chemistry, materials science, continuum mechanics, and computation. The participants from these fields interact with each other through lectures, panel discussions,

group discussions, and poster presentations. The third result is the direct communication of researchers and leading authorities from such governmental agencies as the National Science Foundation (Ken Chong), Army Research Office (Bruce LaMattina), and Department of Energy laboratories (Tomas Diaz de la Rubia and Stephen Zinkle).

In more concrete form, the workshop has resulted in five specific recommendations to governmental agencies and to the community of computational nanomechanics.

The first recommendation concerns the education of engineering students in the United States. This group of participants recommends that elements of nanomechanics be incorporated into existing courses, instead of being created as standalone courses at the undergraduate level. Many of the ingredients of nanomechanics can be included in existing courses, such as Solid Mechanics, Strength of Materials, and Introduction to Engineering Materials. At the graduate level, the flexibility is larger and new courses are feasible – and this is happening on many campuses.

The second recommendation concerns the fabrication of machines from nanostructures. This group of participants recommends that nanomechanics in the fabrication processes deserve concerted effort within the academic community and beyond. Much has been learned over the past decade on individual elements of nanostructures – nanotubes are prime example. However, the fabrication of individual elements into operating machines remains a challenge. Such fabrication requires a fundamental understanding of physics, chemistry, materials, mechanical engineering design, and needless to say, the visionary support of government agencies.

The third recommendation concerns the scale bridging in computational nanomechanics. This group of participants recommends that the time-scale bridging be a focus, as much as the length-scale if not more so. In micro/macro mechanics, the atomic time scale is usually decoupled from that of engineering processes. However, nanostructures' intrinsic vibration time scale can be close to the atomic time scale. As a result, the atomic time scale becomes relevant, and needs to be incorporated into computational mechanics models. Such incorporation remains a challenge.

The fourth recommendation concerns the interface of nanomechanics with biomechanics. This group of participants identifies the interface mechanics of solid nanostructures and biological systems as an important area of research. Intrinsically, nanostructures have large surface areas (relative to volume), and they attract many biological and chemical molecules. This feature enables the use of nanostructures as biological sensors, for example. The mechanical responses of such interfaces depend on the mechanics of both the solids and the molecules. The computational mechanics community is in the position to reach out and tackle this interface issue.

Finally, the fifth recommendation concerns the *sincere* cross fertilization of researchers in physics, chemistry, materials science, continuum mechanics, and computation. Many advanced computational methods are ready to make impacts in nanomechanics research. To realize the impacts, these methods must reach the reality, which is governed by physical principles. If computational methods are like skeletons of humans, physical principles (physics, chemistry, materials science, and continuum mechanics) are the soul of humans. A skeleton functions only when it has a soul. Similarly, a soul has to reside in a skeleton.

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